C^*-ALGEBRAS AND NUMERICAL LINEAR ALGEBRA

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Abstract. Given a self adjoint operator A on a Hilbert space, suppose that that one wishes to compute the spectrum of A numerically. In practice, these problems often arise in such a way that the matrix of A relative to a natural basis is "sparse". For example, doubly infinite tridiagonal matrices are usually associated with discretized second order differential operators. In these cases it is easy and natural to compute the eigenvalues of large $n \times n$ submatrices of the infinite operator matrix, and to hope that if n is large enough then the resulting distribution of eigenvalues will give a good approximation to the spectrum of A.

While this hope is often realized in practice it often fails as well, and it can fail in spectacular ways. The sequence of eigenvalue distributions may not converge as $n \to \infty$, or they may converge to something that has little to do with the original operator A. At another level, even the meaning of 'convergence' has not been made precise in general. In this paper we determine the proper general setting in which one can expect convergence, and we describe the asymptotic behavior of the $n \times n$ eigenvalue distrubutions in all but the most pathological cases. Under appropriate hypotheses we establish a precise limit theorem which shows how the spectrum of A is recovered from the sequence of eigenvalues of the $n \times n$ compressions.

In broader terms, our results have led us to the conclusion that *numerical problems involving infinite dimensional operators require a reformulation in terms of* C^*-algebras. Indeed, it is only when the single operator A is viewed as an element of an appropriate C^*-algebra $\mathcal{A}$ that one can see the precise nature of the limit of the $n \times n$ eigenvalue distributions; the limit is associated with a tracial state on $\mathcal{A}$. Normally, $\mathcal{A}$ is highly noncommutative, and in the main applications it is a simple C^*-algebra having a unique tracial state. We obtain precise asymptotic results for the case where A is the discretized Hamiltonian of a one-dimensional quantum system with arbitrary potential.

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1. Introduction.

There are efficient algorithms available for computing the spectrum of self-adjoint $n \times n$ matrices. Using a good desktop computer, one can find all of the eigenvalues of a 100×100 Toeplitz matrix in a few seconds. It is natural to ask how these finite-dimensional methods might be applied to compute the spectrum of the discretized Hamiltonian of a one dimensional quantum system, or a self-adjoint operator in an irrational rotation C^*-algebra. Considering the burgeoning capabilities of modern computers, it is unfortunate that there are apparently no guidelines available which indicate how one might proceed with such a project except in a few isolated cases. For example, we were unable to determine from the literature if such a program is even *possible* in general.

The purpose of this paper is to develop some general methods for computing the spectrum (more precisely, the essential spectrum) of a self-adjoint operator in terms of the eigenvalues of a sequence of finite dimensional matrix approximations. We will see that there is a natural notion of *degree* of an operator (relative to a filtration of the underlying Hilbert space into finite dimensional subspaces) which generalizes the classical idea of band-limited matrices. More significantly, we will find that this kind of numerical analysis leads one to a broader context, in which the operator is seen as an element of a C^*-algebra which is frequently simple and possesses at least one tracial state. The limit distributions arising from the finite dimensional eigenvalue distributions correspond to traces on this C^*-algebra.

Our intention is not to discuss algorithms *per se*, but rather to present an effective program for utilizing the finite dimensional techniques to compute infinite dimensional spectra, along with a precise description of a broad class of operators for which it will succeed. Thus, we deal with issues arising from operator theory and operator algebras; we do not address questions relating directly to numerical analysis.

In more concrete terms, given an orthonormal basis $\{e_1, e_2, \dots\}$ for a Hilbert space H and an operator $A \in \mathcal{B}(H)$, we may consider the associated infinite matrix (a_{ij})

$$a_{ij} = \langle Ae_j, e_i \rangle, \qquad i, j = 1, 2, \dots,$$

and one can attempt to approximate the spectrum of A by calculating the eigenvalues of large $n \times n$ submatrices

$$A_n = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}.$$

This program fails dramatically in general. For example, if A is the simple unilateral shift (defined on such a basis by $Ae_n = e_{n+1}, n \geq 1$), then the spectrum of A is the closed unit disk and the essential spectrum of A is the unit circle, while $\sigma(A_n) = \{0\}$ for every n because each A_n is a nilpotent matrix.

Examples like this have caused operator theorists to view matrix approximations with suspicion, and to routinely look elsewhere for effective means of computing spectra. On the other hand, since the 1920s there has been evidence that for *self-adjoint* operators, this program can be successfully carried out.

Consider for example the following theorem of Szegö. Let f be a *real* function in $L^\infty[-\pi,\pi]$ and let A be the multiplication operator

$$A\xi(x) = f(x)\xi(x), \qquad \xi \in L^2[-\pi,\pi].$$

With respect to the familiar orthonormal basis $\{e_n : n \in \mathbb{Z}\}$, $e_n(x) = e^{inx}$, the matrix of A is a doubly-infinite Laurent matrix whose principal $n \times n$ submatrices are finite self-adjoint Toeplitz matrices

$$A_n = \begin{pmatrix} a_0 & a_{-1} & \dots & a_{-n+1} \\ a_1 & a_0 & \dots & a_{-n+2} \\ \vdots & & \ddots & \vdots \\ a_{n-1} & \dots & & a_0 \end{pmatrix},$$

the numbers a_k being the Fourier coefficients of f. Let $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ be the eigenvalues of A_n, repeated according to multiplicity. Szegö's theorem asserts that for every continuous function $u : \mathbb{R} \to \mathbb{R}$ we have

1.1 $$\lim_{n\to\infty} \frac{1}{n}(u(\lambda_1) + u(\lambda_2) + \dots + u(\lambda_n)) = \frac{1}{2\pi}\int_{-\pi}^{\pi} u(f(x))\, dx.$$

See [8][10]; a discussion of Szegö's theorem can be found in [11], and [6] contains a meticulous discussion of Toeplitz operators.

Let us reformulate Szegö's theorem in terms of weak*-convergence of measures. Let a and b be the essential inf and essential sup of f

$$a = \operatorname*{ess\,inf}_{-\pi\le x\le\pi} f(x)$$
$$b = \operatorname*{ess\,sup}_{-\pi\le x\le\pi} f(x),$$

and let μ be the probability measure defined on $[a,b]$ by

$$\mu(S) = \frac{1}{2\pi} m\{x : f(x) \in S\},$$

m denoting Lebesgue measure on $[-\pi,\pi]$. Then 1.1 asserts that the sequence of discrete probability measures

$$\mu_n = \frac{1}{n}(\delta_{\lambda_1} + \delta_{\lambda_2} + \dots + \delta_{\lambda_n}),$$

δ_λ denoting the unit point mass at λ, converges to μ in the weak*-topology of the dual of $C[a,b]$,

$$\lim_{n\to\infty} \int_a^b u(x)\, d\mu_n(x) = \int_a^b u(x)\, d\mu(x), \qquad u \in C[a,b].$$

The spectrum of A coincides with its essential spectrum in this case, and is exactly the closed support of the measure μ.

Once one knows that the measures μ_n converge in this way to a measure supported exactly on $\sigma_e(A)$, one may draw rather precise conclusions about the rate

at which the eigenvalues of A_n accumulate at points of the essential spectrum. For example, suppose that we choose a point $\lambda \in \sigma_e(A)$. Then for every open interval I containing λ we have $\mu(I) > 0$. If we choose positive numbers α and β which are close to $\mu(I)$ and satisfy $\alpha < \mu(I) < \beta$, then in the generic case where A has no point spectrum we may conclude that

$$n\alpha < \#(\sigma(A_n) \cap I) < n\beta$$

when n is sufficiently large. Of course, the symbol # means the number of eigenvalues in the indicated set, counting repeated eigenvalues according to the multiplicity of their occurrence. In a similar way, the density of eigenvalues of A_n tends to become increasingly sparse around points of the complement of the essential spectrum.

In this paper we will show that, while convergence of this type cannot be expected in general, it does persist in a much broader context than the above. Actually, this work was initiated in order to develop methods for computing the essential spectrum of certain tridiagonal operators which are associated with the discretized Hamiltonians of one-dimensional quantum mechanical systems (see section 5). These operators serve to illustrate the flavor of our more general results. Starting with a real valued continuous function V of a real variable, we fix a real number θ and consider the tridiagonal operator T defined in terms of a bilateral orthonormal basis $\{e_n : n \in \mathbb{Z}\}$ by

$$Te_n = e_{n-1} + d_n e_n + e_{n+1},$$

where the diagonal sequence is defined by $d_n = V(\sin(n\theta))$, $n \in \mathbb{Z}$. The compression T_n of T to the span of $\{e_k : -n \leq k \leq n\}$ is a $(2n+1) \times (2n+1)$ tridiagonal matrix whose eigenvalues can be computed very rapidly using modern algorithms. For example, we show that if μ_n is the discrete probability measure defined by the eigenvalue distribution of T_n,

$$\mu_n = \frac{1}{2n+1}(\delta_{\lambda_1} + \delta_{\lambda_2} + \dots \delta_{\lambda_{2n+1}}),$$

then there is a probability measure μ *having closed support* $\sigma_e(T)$, such that for every continuous function $f : \mathbb{R} \to \mathbb{R}$ we have

$$\lim_{n\to\infty} \int f(x)\, d\mu_n(x) = \int f(x)\, d\mu(x).$$

See formula 5.1.

In these cases the limiting measure μ can be identified in rather concrete terms. Briefly, if θ/π is irrational then the pair of unitary operators

$$Ue_n = e_{n+1}$$
$$Ve_n = e^{in\theta} e_n$$

generate an irrational rotation C^*-algebra $\mathcal{A}_\theta$. $\mathcal{A}_\theta$ has an essentially unique representation in which its weak closure is the II_1 factor R. T becomes a self-adjoint operator in R, and the measure μ is defined by

$$\mu(S) = \tau(E_T(S)), \qquad S \subseteq \mathbb{R}$$

where τ is the normalized trace on R and E_T is the spectral measure of T.

In sections 2 and 3 we consider a rather general question. Given a self-adjoint operator A and an orthonormal basis for the underlying Hilbert space, let (a_{ij}) be the matrix of A relative to this basis. How must one choose the basis so that the essential spectrum of A can be computed *in principle* from the eigenvalues of the finite dimensional principal submatrices of (a_{ij})? Roughly speaking, we show that this is possible if the diagonals of the matrix (a_{ij}) tend to zero sufficiently fast. It is *not* possible in general. The family of all operators whose matrices satisfy this growth condition is a Banach $*$-algebra but it is not a C^*-algebra.

In section 4 we seek more precise results which relate to weak*-convergence as above. It is appropriate to formulate these results in terms of C^*-algebras of operators. We introduce the notion of *degree* of an operator (relative to a filtration of the underlying Hilbert space into finite dimensional subspaces), and show that one can expect convergence of this type in the state space of the given C^*-algebra when the C^*-algebra contains a dense set of finite degree operators and has a unique tracial state. These results are applied in section 5 to the discretized Hamiltonians described above.

2. Spectral asymptotics of sequences of matrices.

Let A be a bounded self-adjoint operator on a Hilbert space H and suppose that we have a sequence of finite-dimensional subspaces H_n of H with the property that the corresponding sequence of projections $P_n \sim H_n$ converges strongly to the identity. Normally, the subspaces H_n will be increasing with n, the main examples arising in the cases where we start with an orthonormal basis $\{e_n : n = 1, 2, \dots\}$ (resp. $\{e_n : n \in \mathbb{Z}\}$) and choose $H_n = [e_1, e_2, \dots, e_n]$ (resp. $H_n = [e_{-n}, e_{-n+1}, \dots, e_n]\}$).

For every $n \geq 1$, let A_n denote the compression

2.1 $$A_n = P_n A|_{H_n}.$$

More generally, given an arbitrary sequence $A_1, A_2, \dots$ of finite dimensional self-adjoint operators, we introduce two "spectral" invariants Λ, Λ_e of the sequence as follows. Λ is defined as the set of all $\lambda \in \mathbb{R}$ with the property that there is a sequence $\lambda_1, \lambda_2, \dots$ such that $\lambda_n \in \sigma(A_n)$ and

$$\lim_{n \to \infty} \lambda_n = \lambda.$$

Notice that Λ *is closed*. Indeed, a real number λ belongs to the complement of Λ iff there is an open set U containing λ and an infinite sequence of integers $n_1 < n_2 < \dots$ with the property that $\sigma(A_{n_k}) \cap U = \emptyset$ for every $k = 1, 2, \dots$. Every point of U shares this property with λ, and hence the complement of Λ is open. If the sequence $\{A_n\}$ is bounded in norm then Λ is compact. Of course, Λ is considerably smaller than the set

$$L = \cap_n \overline{(\sigma(A_n) \cup \sigma(A_{n+1}) \cup \dots)}$$

of limit points of the sequence $\sigma(A_1), \sigma(A_2), \dots$, since limits along subsequences may not qualify for membership in Λ.

For every $n \geq 1$ and every set S of real numbers, let $N_n(S)$ be the number of eigenvalues of A_n which belong to S, counting multiple eigenvalues according to their multiplicity. $N_n(\cdot)$ is an integer-valued measure which takes values $0, 1, 2, \dots, \dim H_n$. The points of Λ are classified as follows.

Definition 2.2.

(1) A point $\lambda \in \mathbb{R}$ is called essential if, for every open set U containing λ, we have
$$\lim_{n\to\infty} N_n(U) = \infty.$$
The set of essential points is denoted Λ_e.

(2) $\lambda \in \mathbb{R}$ is called transient if there is an open set U containing λ such that
$$\sup_{n\geq 1} N_n(U) < \infty.$$

Remarks. It is clear that $\Lambda_e \subseteq \Lambda$. Moreover, notice that $\lambda \in \mathbb{R}$ is nonessential iff there is an open set U containing λ and an infinite sequence of integers $n_1 < n_2 < \dots$ such that
$$N_{n_k}(U) \leq M < \infty$$
for every $k = 1, 2, \dots$. Thus the nonessential points are an open set in $\mathbb{R}$, and we conclude that *the set Λ_e of essential points is closed*.

It is conceivable that Λ may contain anomalous points which are neither transient nor essential. In small neighborhoods U of such a point one would find subsequences n_k for which $N_{n_k}(U)$ remains bounded, and other subsequences m_k for which $N_{m_k}(U)$ is unbounded. Fortunately, in most situations one has a more manageable dichotomy (see Theorem 3.8). At this level of generality, one cannot say much. We do have the following

Theorem 2.3. *Assuming that the sequence $A_1, A_2, \dots$ arises from an operator A as in 1.1, then we have $\sigma(A) \subseteq \Lambda$ and $\sigma_e(A) \subseteq \Lambda_e$.*

proof of $\sigma(A) \subseteq \Lambda$.

Suppose that λ is a real number which does not belong to Λ. We will show that $A - \lambda\mathbf{1}$ is invertible. Since $\lambda \notin \Lambda$, there is an $\epsilon > 0$ and a subsequence $n_1 < n_2 < \dots$ such that
$$\sigma(A_{n_k}) \cap (\lambda - \epsilon, \lambda + \epsilon) = \emptyset$$
for every $k \geq 1$. Thus the distance from λ to $\sigma(A_{n_k})$ is at least ϵ, hence
$$\| (A_{n_k} - \lambda\mathbf{1})^{-1} \| \leq 1/\epsilon$$
for every k. Let
$$B_k = (A_{n_k} - \lambda\mathbf{1})^{-1} P_{n_k}.$$
Since $B_1, B_2, \dots$ is a bounded sequence of self-adjoint operators and the ball of $\mathcal{B}(H)$ of radius $1/\epsilon$ is weakly sequentially compact, $\{B_k\}$ has a weakly convergent subsequence. Thus, by replacing the original sequence $n_1, n_2, \dots$ with a subsequence of itself, we may assume that there is a bounded operator B such that
$$\lim_{k\to\infty} < B_k\xi, \eta > = < B\xi, \eta >, \qquad \xi, \eta \in H.$$

Since

2.4 $$(A_{n_k} - \lambda\mathbf{1})B_k = P_{n_k}$$

for every k and since $(A_{n_k} - \lambda\mathbf{1})P_{n_k}$ converges to $A - \lambda\mathbf{1}$ in the *strong* operator topology, it follows that the product $(A_{n_k} - \lambda\mathbf{1})B_{n_k}$ converges weakly to $(A - \lambda\mathbf{1})B$. Hence from 2.4 we may conclude that

$$(A - \lambda\mathbf{1})B = \operatorname{weak}\lim_{k\to\infty} P_{n_k} = \mathbf{1},$$

proving that $A - \lambda\mathbf{1}$ is right-invertible. Left-invertiblity follows by taking adjoints in the preceding equation.

proof of $\sigma_e(A) \subseteq \Lambda_e$.

Suppose that $\lambda \notin \Lambda_e$. We will show that $A - \lambda\mathbf{1}$ is invertible modulo trace class operators, and hence $\lambda \notin \sigma_e(A)$. By the hypothesis on λ, there is a sequence $n_1 < n_2 < \dots$ of positive integers and a pair of positive numbers ϵ, M such that

$$N_{n_k}(\lambda - \epsilon, \lambda + \epsilon) \leq M$$

for every $k = 1, 2, \dots$. For each k, consider A_{n_k} to be a self-adjoint operator in $\mathcal{B}(P_{n_k}H)$ and let E_k be the spectral measure of this operator. Then $Q_k = E_k(\lambda - \epsilon, \lambda + \epsilon)$ is a projection commuting with A_{n_k} satisfying $\dim Q_k \leq M$, such that the restriction B_k of $A_{n_k} - \lambda\mathbf{1}$ to the range of $P_{n_k} - Q_k$ is an invertible operator with $\| B_k^{-1} \| \leq 1/\epsilon$.

By using compactness again and passing to a subsequence as in the preceding argument, we can assume that both sequences $\{B_k^{-1}(P_{n_k} - Q_k)\}$ and $\{Q_k\}$ converge in the weak operator topology

$$B_k^{-1}(P_{n_k} - Q_k) \to C$$
$$Q_k \to Q.$$

Notice that Q is a positive trace class operator. Indeed, since the set

$$\{T \in \mathcal{B}(H) : T \geq 0, \operatorname{trace}(T) \leq M\}$$

is closed in the weak operator topology, the assertion is evident. Finally, using the fact that $A_{n_k} - \lambda\mathbf{1}$ converges in the *strong* operator topology to $A - \lambda\mathbf{1}$ and

$$(A_{n_k} - \lambda\mathbf{1})B_k^{-1}(P_{n_k} - Q_k) = P_{n_k} - Q_k$$

for every k, we may take weak limits in the latter formula to obtain

$$(A - \lambda\mathbf{1})C = \mathbf{1} - Q,$$

as required $\square$

Remarks. The appendix contains an example which shows that the inclusions of Theorem 2.3 can be proper.

One can imagine computing the eigenvalues of A_n for every $n = 1, 2, \dots$, picking a point $\lambda \in \Lambda$, and observing the distribution of eigenvalues in the vicinity of λ as n becomes large. If λ is essential then the number of eigenvalues in any small interval containing λ will increase without limit. If λ is transient, then there are positive integers $p \leq q$ with the property that eventually you always see at least p points in the interval but never more than q. Moreover, after p and q are appropriately adjusted, then the same behavior will occur in *every* sufficiently small interval containing λ.

3. Filtrations and their Banach algebras.

Let A be a self adjoint operator on a Hilbert space H. Suppose we have an orthonormal basis for H, indexed either by $\mathbb{N}$ or $\mathbb{Z}$, and we form the matrix (a_{ij}) of A relative to this basis. If we form a sequence of finite-dimensional compressions of (a_{ij}) then we may compute Λ and Λ_e in principle, and the general results of section 2 imply that $\sigma_e(A) \subseteq \Lambda_e$. In this section we find conditions on the matrix (a_{ij}) which guarantee first, that every point of Λ is either essential or transient and second, that $\sigma_e(A) = \Lambda_e$. The criterion is that the series $\sum_k |k|^{1/2} d_k$ should converge, where d_k is the sup norm of the kth diagonal of (a_{ij}). We conclude this section with some comments about the nature of transient points.

In order to deal with both unilateral and bilateral orthonormal bases as well as more general situations in which the dimensions of compressions increase in uneven jumps, it is necessary to work with filtrations. We introduce the concept of *degree* of an operator and a Banach $*$-algebra $D(\mathcal{F})$ of operators associated with a filtration $\mathcal{F}$. It is important for the applications that it should be easy to estimate the norm in $D(\mathcal{F})$ (see Proposition 3.4).

Definition 3.1.

(1) A *filtration* of H is a sequence $\mathcal{F} = \{H_1, H_2, \dots\}$ of finite dimensional subspaces of H such that $H_n \subseteq H_{n+1}$ and

$$\overline{\cup_n H_n} = H.$$

(2) Let $\mathcal{F} = \{H_n\}$ be a filtration of H and let P_n be the projection onto H_n. The *degree* of an operator $A \in \mathcal{B}(H)$ is defined by

$$\deg(A) = \sup_{n \geq 1} \operatorname{rank}(P_n A - A P_n).$$

Remarks. $\deg(A)$ is either a nonnegative integer or $+\infty$. Moreover, we have

$$\deg(A^*) = \deg(A), \quad \deg(\lambda A) = \deg(A) \ \textit{for all}\ \lambda \neq 0,$$
$$\deg(A + B) \leq \deg(A) + \deg(B), \quad \deg(AB) \leq \deg(A) + \deg(B).$$

Only the last of the four properties is not quite obvious; it follows from the fact that the map $A \to [P_n, A] = P_n A - A P_n$ is a derivation, $[P_n, AB] = [P_n, A]B + A[P_n, B]$, which implies

$$\operatorname{rank}[P_n, AB] \leq \operatorname{rank}[P_n, A] + \operatorname{rank}[P_n, B].$$

We conclude from these observations that the set of all finite-degree operators in $\mathcal{B}(H)$ is a self-adjoint unital subalgebra of $\mathcal{B}(H)$.

Remark. Notice that for any operator A and any projection P we have

$$PA - AP = PA(\mathbf{1} - P) - (\mathbf{1} - P)AP,$$

hence

$$\operatorname{rank}(PA - AP) = \operatorname{rank}(PA(\mathbf{1} - P)) + \operatorname{rank}((\mathbf{1} - P)AP)$$
$$= \operatorname{rank}((\mathbf{1} - P)A^*P) + \operatorname{rank}((\mathbf{1} - P)AP)$$

It follows that $\deg(A) < \infty$ iff both operators $B = A$ and $B = A^*$ satisfy the condition

$$\sup_{n\geq 1} \operatorname{rank}((\mathbf{1} - P_n)BP_n) < +\infty.$$

Thus, *operators of finite degree are abstractions of band-limited matrices.*

We associate a Banach $*$-algebra $D(\mathcal{F})$ to a filtration $\mathcal{F}$ in the following way. Let $D(\mathcal{F})$ denote the set of all operators $A \in \mathcal{B}(H)$ having a decomposition into an infinite sum of finite degree operators A_k

$$A = \sum_{k=1}^{\infty} A_k \tag{3.2}$$

in such a way that the sum

$$s = \sum_{k=1}^{\infty} (1 + \deg(A_k)^{1/2})\|A_k\|$$

is finite. Notice that finiteness of s ensures that the series 3.2 converges absolutely with respect to the operator norm. We define $|A|_{\mathcal{F}}$ to be the infimum of all such sums s which arise from representations of A as in 3.2.

Proposition 3.3. *With respect to the norm $|\cdot|_{\mathcal{F}}$ and the operator adjoint, $D(\mathcal{F})$ is a unital Banach $*$-algebra in which $|\mathbf{1}|_{\mathcal{F}} = 1$.*

proof. Let $\mathcal{D}$ be the $*$-algebra of all finite degree operators in $\mathcal{B}(H)$, and consider the function $\phi : \mathcal{D} \to \mathbb{R}^+$ defined by

$$\phi(A) = (1 + (\deg A)^{1/2})\|A\|.$$

The norm on $D(\mathcal{F})$ is defined by

$$|A|_{\mathcal{F}} = \inf \sum_{k=1}^{\infty} \phi(A_k),$$

the infimum extended over all sequences $A_1, A_2, \dots$ in $\mathcal{D}$ satisfying

$$A = \sum_{k=1}^{\infty} A_k$$

together with $\sum_k \phi(A_k) < +\infty$. The fact that $(D(\mathcal{F}), |\cdot|_{\mathcal{F}})$ is a Banach $*$-algebra follows from straightforward applications of the following properties of ϕ:

(1) $\phi(A) \geq \|A\|$.
(2) $\phi(\lambda A) = |\lambda| \cdot \|A\|, \quad \lambda \in \mathbb{C}$.
(3) $\phi(A^*) = \phi(A)$.
(4) $\phi(AB) \leq \phi(A)\phi(B)$.

For example, (4) follows from the fact that the weight sequence $w_0, w_1, w_2, \dots$ defined by $w_k = 1 + k^{1/2}$ satisfies

$$w_{k+j} \leq w_k w_j, \qquad k, j \geq 0,$$

together with

$$\deg(AB) \leq \deg A + \deg B.$$

The identity of $\mathcal{B}(H)$ is of degree 0, hence $|\mathbf{1}|_{\mathcal{F}} \leq 1$, while the inequality $|\mathbf{1}|_{\mathcal{F}} \geq 1$ is valid for the unit of any Banach algebra $\square$

$D(\mathcal{F})$ is certainly not a C^*-algebra, but it is dense in $\mathcal{B}(H)$ in the strong operator topology. The following gives a concrete description of operators in $D(\mathcal{F})$ for one of the two most important filtrations

Proposition 3.4. *Let $\{e_n : n \in \mathbb{Z}\}$ be a bilateral orthonormal basis for a Hilbert space H and let $\mathcal{F} = \{H_1, H_2, \dots\}$ be the filtration defined by*

$$H_n = [e_{-n}, e_{-n+1}, \dots, e_n].$$

Let (a_{ij}) be the matrix of an operator $A \in \mathcal{B}(H)$ relative to $\{e_n\}$, and for every $k \in \mathbb{Z}$ let

$$d_k = \sup_{i \in \mathbb{Z}} |a_{i+k,i}|$$

be the sup norm of the kth diagonal of (a_{ij}). Then

$$|A|_{\mathcal{F}} \leq \sum_{k=-\infty}^{+\infty} (1 + |2k|^{1/2}) d_k. \tag{3.5}$$

In particular, A will belong to $D(\mathcal{F})$ whenever the series $\sum_k |k|^{1/2} d_k$ converges.

proof. We may assume that the sum on the right side of 3.5 converges. Let D_k be the operator whose matrix agrees with (a_{ij}) along the kth diagonal and is zero elsewhere. Notice that $||D_k|| = d_k$, and hence

$$A = \sum_{k=-\infty}^{+\infty} D_k,$$

the sum on the right converging absolutely in the operator norm because

$$\sum_k |k|^{1/2} d_k < \infty.$$

We claim that $\deg D_k \leq 2|k|$ for every $k \in \mathbb{Z}$. To see that, fix $n = 1, 2, \dots$ and let P_n be the projection onto H_n. The operator D_k maps the range of P_n into the range of $P_{n+|k|}$, and a careful inspection of the two cases $k > 0$ and $k < 0$ shows that the dimension of $(\mathbf{1} - P_n)P_{n+|k|}$ is at most $|k|$ for every $n \geq 1$. It follows that the rank of either operator $(\mathbf{1} - P_n)D_k P_n$ or $(\mathbf{1} - P_n)D_k^* P_n$ is at most $|k|$, independently of n. Thus from a previous remark we conclude that $\deg D_k \leq 2|k|$.

Now $\|D_k\| = d_k$, and since the series $\sum_k |k|^{1/2} d_k$ converges we must have $\sum_k \|D_k\| < \infty$. Hence

$$A = \sum_{k=-\infty}^{+\infty} D_k$$

is an absolutely convergent sum of operators D_k satisfying $\deg D_k \leq 2|k|$, from which 3.5 follows $\square$

In particular, any operator whose matrix (a_{ij}) is *band-limited* in the sense that $a_{ij} = 0$ whenever $|i - j|$ is sufficiently large, must belong to $D(\mathcal{F})$.

The following estimate occupies a key position, and it explains why the norm on $D(\mathcal{F})$ is defined as it is. For $B \in \mathcal{B}(H)$, we write $\|B\|_2 = (\mathrm{trace}(B^*B))^{1/2}$ for the Hilbert-Schmidt norm of B.

Lemma 3.6. *Let $\{H_1, H_2, \dots\}$ be a filtration of H and let P_n be the projection onto H_n. Then for every $A \in D(\mathcal{F})$ we have*

$$\sup_{n\geq 1} \|AP_n - P_nAP_n\|_2 \leq |A|_{\mathcal{F}} < \infty.$$

proof. We claim first that for every $A \in \mathcal{B}(H)$ and every $n = 1, 2, \dots$ we have

$$\text{trace}|AP_n - P_nAP_n|^2 \leq \deg(A)\|A\|^2, \tag{3.7}$$

where for an operator $B \in \mathcal{B}(H)$, $|B|$ denotes the positive square root of B^*B. Indeed, since $\text{trace}|B|^2 \leq \text{rank}(B)\|B\|^2$, we can estimate the left side of 3.7 as follows

$$\begin{aligned}\text{trace}|(\mathbf{1} - P_n)AP_n|^2 &\leq \text{rank}((\mathbf{1} - P_n)AP_n))\|(\mathbf{1} - P_n)AP_n\|^2 \\ &= \text{rank}((\mathbf{1} - P_n)(AP_n - P_nA))\|(\mathbf{1} - P_n)AP_n\|^2 \\ &\leq \text{rank}(AP_n - P_nA)\|A\|^2 \leq \deg(A)\|A\|^2.\end{aligned}$$

By taking the square root of both sides of 3.7 we obtain

$$\|AP_n - P_nAP_n\|_2 \leq \deg(A)^{1/2}\|A\|.$$

Now suppose $A \in D(\mathcal{F})$, and choose finite degree operators A_k such that

$$\sum_k (1 + \deg(A_k)^{1/2})\|A_k\| < \infty$$

and $A = A_1 + A_2 + \dots$. Using the triangle inequality for the Hilbert-Schmidt norm we see from 3.7 that

$$\begin{aligned}\|P_nA - P_nAP_n\|_2 &\leq \sum_{k=1}^{\infty} \deg(A_k)^{1/2}\|A_k\| \\ &\leq \sum_{k=1}^{\infty} (1 + \deg(A_k)^{1/2})\|A_k\|.\end{aligned}$$

The desired inequality follows by taking the supremum over n and the infimum over all such sequences $A_1, A_2, \dots$ □

Remark. Notice that Lemma 3.6 implies that for every $A \in D(\mathcal{F})$ we have the following uniform estimate of commutator 2-norms

$$\sup_n \|AP_n - P_nA\|_2 \leq \sqrt{2}|A|_{\mathcal{F}} < +\infty.$$

Now let A be a self-adjoint operator in $\mathcal{B}(H)$, let $\mathcal{F} = \{H_1, H_2, \dots\}$ be a filtration, and let A_n be the compression of A to H_n. The following result is our basic description of the spectrum of A in terms of the eigenvalues of $\{A_n\}$. It asserts that the essential spectrum of A is precisely the set of essential points, and that all of the remaining points of A are transient.

Theorem 3.8. *Assume that $A = A^*$ belongs to the Banach algebra $D(\mathcal{F})$. Then*

(i) $\sigma_e(A) = \Lambda_e$.

(ii) *Every point of Λ is either transient or essential.*

proof. We will prove that every point in the complement of the essential spectrum of A is transient. Notice that both statements (i) and (ii) follow from this. Indeed, because of Theorem 2.3 we know that $\sigma_e(A) \subseteq \Lambda_e$. On the other hand, since no transient point can be an essential point, the above assertion implies that the complement of $\sigma_e(A)$ is contained in the complement of Λ_e; hence (i). Armed with (i), we see that $\Lambda \setminus \Lambda_e$ is the same as $\Lambda \setminus \sigma_e(A)$, which by the assertion is contained in the transient points of Λ. Thus we obtain (ii).

To prove this assertion, choose a point λ in the complement of $\sigma_e(A)$. In order to show that λ is transient, we claim first that there is a finite-dimensional projection Q and a positive number ϵ such that for every real number $\mu \in [\lambda - \epsilon, \lambda + \epsilon]$, the operator

$$A + Q - \mu\mathbf{1}$$

is invertible. Indeed, since $\lambda \notin \sigma_e(A)$ it follows that either λ is an isolated point of the spectrum of A whose eigenspace is finite dimensional, or else $A - \lambda\mathbf{1}$ is invertible. In either case

$$\{\xi \in H : A\xi = \lambda\xi\}$$

is finite dimensional and if Q denotes the projection onto this eigenspace, then Q commutes with A and $A + Q - \lambda\mathbf{1}$ is an invertible self-adjoint operator. Because the invertible operators are an open set it follows that there is a neighborhood U of λ with the property that $A + Q - \mu\mathbf{1}$ is invertible for every $\mu \in U$. We can take $[\lambda - \epsilon, \lambda + \epsilon]$ to be an appropriate closed interval about λ which is contained in such a neighborhood.

Note too that by continuity of inversion, there is a positive number M such that

$$\| (A + Q - \mu\mathbf{1})^{-1} \| \leq M \tag{3.9}$$

for every μ satisfying $|\mu - \lambda| \leq \epsilon$.

We will show that if V is the open interval $(\lambda - \epsilon, \lambda + \epsilon)$ and $N_n(V)$ is the number of eigenvalues of A_n which lie in V, then the sequence $N_n(V)$ is bounded. Thus λ must be a transient point, and that will complete the proof. To that end, note first that by Lemma 3.6 there is a positive number N (in fact, $N = |A|^2_{\mathcal{F}}$ will do) such that

$$\operatorname{trace}|AP_n - P_nAP_n|^2 \leq N,$$

for every $n = 1, 2, \dots$. Fix n, and let $\lambda_1, \lambda_2, \dots, \lambda_p$ be the set of all eigenvalues of A_n which lie in V, with repetitions according to the multiplicity of the corresponding eigenspace. Actually, we will show that

$$p \leq M^2 N + \dim Q. \tag{3.10}$$

Since the right side of 3.10 does not depend on n it will follow that λ is transient, completing the proof.

To prove 3.10, we choose for each $k = 1, 2, \dots, p$ a unit vector ξ_k in the domain of A_n (i.e., the range of P_n) such that $A_n\xi_k = \lambda_k\xi_k$, and such that $\{\xi_1, \dots, \xi_p\}$ is an orthonormal set. This is possible because the eigenvectors which belong to

different eigenvalues of a self-adjoint operator are mutually orthogonal; in the case of a multiple eigenvalue we simply choose an orthonormal basis for that eigenspace.

Note first that for each k between 1 and p,

$$A\xi_k - \lambda_k \xi_k = (\mathbf{1} - P_n) A\xi_k. \tag{3.11}$$

Indeed, since $P_n(A\xi_k - \lambda_k\xi_k) = A_n\xi_k - \lambda_k\xi_k = 0$, we can write

$$A\xi_k - \lambda_k\xi_k = (\mathbf{1} - P_n)(A\xi_k - \lambda_k\xi_k) = (\mathbf{1} - P_n)A\xi_k.$$

We claim now that for each k between 1 and p, we have the inequality

$$1 \leq M^2 \parallel (\mathbf{1} - P_n)A\xi_k \parallel^2 + < Q\xi_k, \xi_k > . \tag{3.12}$$

To see that, write

$$\begin{aligned} 1- < Q\xi_k, \xi_k > &= \parallel (\mathbf{1} - Q)\xi_k \parallel^2 \leq \ M^2 \parallel (A + Q - \lambda_k)(\mathbf{1} - Q)\xi_k \parallel^2 \\ &= M^2 \parallel (A - \lambda_k \mathbf{1})(\mathbf{1} - Q)\xi_k \parallel^2 = \parallel (\mathbf{1} - Q)(A\xi_k - \lambda_k\xi_k) \parallel \\ &= M^2 \parallel (\mathbf{1} - Q)(\mathbf{1} - P_n)A\xi_k \parallel^2 \leq \ M^2 \parallel (\mathbf{1} - P_n)A\xi_k \parallel^2 . \end{aligned}$$

The first inequality follows from 3.9, the identity $(A-\lambda_k)(\mathbf{1}-Q)\xi_k = (\mathbf{1}-Q)(A\xi_k - \lambda_k\xi_k)$ follows from the fact that Q and A commute, and the last equality and inequality follow respectively from 3.11 and the fact that $\mathbf{1} - Q$ is a contraction. Summing the inequality 3.12 on k we obtain

$$\begin{aligned} p &\leq M^2 \sum_{k=1}^{p} \parallel (\mathbf{1} - P_n)A\xi_k \parallel^2 + \sum_{k=1}^{p} < Q\xi_k, \xi_k > \\ &\leq M^2 \,\mathrm{trace}|(\mathbf{1} - P_n)AP_n|^2 + \mathrm{trace}(Q) \\ &\leq M^2 N + \mathrm{dim} Q, \end{aligned}$$

and 3.10 is established □

Remark 3.13. We conclude this section with some remarks about transient points and other spurious eigenvalues. To provide a context for these remarks, let us return to the classical setting of Szegö's theorem, in which $A_1, A_2, \ldots$ is a sequence of Toeplitz matrices. Let f be a bounded measurable real-valued function on the interval $[-\pi, \pi]$, and consider the Fourier series of f

$$f(x) \sim \sum_{n=-\infty}^{\infty} a_n e^{inx}.$$

For $n = 1, 2, \ldots$ let A_n be the Toeplitz matrix

$$A_n = \begin{pmatrix} a_0 & a_{-1} & \ldots & a_{-n+1} \\ a_1 & a_0 & \ldots & a_{-n+2} \\ \vdots & & \ddots & \vdots \end{pmatrix}.$$

Let a and b be respectively the essential inf and sup of f over $[\pi, \pi]$. It is known that the eigenvalues of the sequence $\{A_n : n = 1, 2, \dots\}$ tend to fill out the entire interval $[a, b]$ (see [11, pp 201–202] and [12, Lemma II.1]). In more concrete terms, suppose that $\lambda \in (a, b)$ and that we are looking in a small neighborhood $U = (\lambda - \epsilon, \lambda + \epsilon)$ of λ. Then $U \cap \sigma(A_n) \neq \emptyset$ for sufficiently large n, regardless of where λ is located in the interval (a, b). The point we want to make is that this can be misleading, and that what one is observing here may have nothing to do with the spectrum of the operator A.

Indeed, for these operators A we have

$$\sigma(A) = \sigma_e(A) = R,$$

where R is the essential range of the function f. Suppose that f is chosen so that its essential range is disconnected. If we choose a point $\lambda \in [a, b] \setminus R$ then for every $\epsilon > 0$ we will find the sets of eigenvalues $(\lambda - \epsilon, \lambda + \epsilon) \cap \sigma(A_n)$ to be permanently nonempty for large n, in spite of the fact that $(\lambda - \epsilon, \lambda + \epsilon)$ contains no points of the spectrum of A if ϵ is small.

Returning to the context of Theorem 3.8, it is not hard to give examples of band-limited matrices (a_{ij}) which exhibit the same kind of behavior, namely $\sigma(A) = \sigma_e(A)$ while Λ contains points not in the spectrum of the operator. In this case, 3.8 implies that such points will be transient. More generally, if one starts with a band-limited operator whose spectrum is properly larger than its essential spectrum, then every point of $\sigma(A) \setminus \sigma_e(A)$ will be a transient point (Theorem 3.8). Of course, for such an operator there may also be other transient points which do *not* belong to $\sigma(A)$. Unfortunately, we do not know how to distinguish between transient points which belong to the spectrum and transient points which do not. Perhaps it is not even possible to do so. In any case, these observations have led us to the conclusion that *transient points should be ignored.* In doing that one is also ignoring points of $\sigma(A) \setminus \sigma_e(A)$; but since such points are merely isolated eigenvalues having finite multiplicity, the cost is small.

We conclude that if one is interested in approximating spectra of infinite dimensional operators using matrix truncations, then one should not simply look for the eigenvalues of the truncations. Rather, *one should weight the count of eigenvalues in a way which eliminates spurious ones occuring in the vicinity of transient points.* The simplest example of such weighting is the sequence of ‘densities’

$$\frac{N_n(U)}{n},$$

where $N_n(U)$ is the number of eigenvalues of the $n \times n$ truncation of A which belong to the open set U. Indeed, in the present context we obviously have

$$\lim_{n \to \infty} \frac{N_n(U)}{n} = 0$$

whenever U is a sufficiently small neighborhood of a transient point λ, simply because the sequence $N_1(U), N_2(U), \dots$ is bounded. If λ is an essential point on the other hand, then we require conditions under which the limit

$$\lim \frac{N_n(U)}{}$$

exists and is positive for every open neighborhood U of λ. The existence of this limit in the case of the multiplication operators A discussed above is a consequence of Szegö's theorem, as we have pointed out in the introduction. In the following section we take up the asymptotic behavior of these densities in a more general context.

4. Filtrations and convergence of densities.

In this section we shift our point of view somewhat. Rather than consider single self-adjoint operators we consider a concretely presented C^*-algebra of operators $\mathcal{A} \subseteq \mathcal{B}(H)$ and we introduce the concept of an $\mathcal{A}$-filtration. This is an abstraction of an orthonormal basis for H with respect to which a dense set of the operators in $\mathcal{A}$ are band-limited. The point we want to make is that in order to use the methods of this paper to compute the spectrum of a self-adjoint operator in a C^*-algebra $\mathcal{C}$, one should first look for a faithful representation $\pi : \mathcal{C} \to \mathcal{B}(H)$ with the property that the C^*-algebra $\mathcal{A} = \pi(\mathcal{C})$ admits a natural $\mathcal{A}$-filtration, and then proceed with the analysis associated with Theorem 3.8 or Theorem 4.5 below.

After presenting some examples, we prove a counterpart of Szegö's theorem which is appropriate for C^*-algebras. In order to keep the statement and proof as simple as possible, we assume that the C^*-algebra has a unique trace. While this is not the most general formulation possible, it does provide the basis for the applications which will be taken up in the next section. It will be convenient (though not necessary) to assume that C^*-algebras of operators on H contain the identity of $\mathcal{B}(H)$.

Definition 4.1. Let $\mathcal{A} \subseteq \mathcal{B}(H)$ be a C^*-algebra. An $\mathcal{A}$-filtration is a filtration of H with the property that the $*$-subalgebra of all finite degree operators in $\mathcal{A}$ is norm-dense in $\mathcal{A}$.

Example 1. The simplest example is that in which $\mathcal{A}$ is an AF-algebra having a cyclic vector ξ. If $\mathcal{A}_1 \subseteq \mathcal{A}_2 \subseteq \dots$ is a sequence of finite dimensional *-subalgebras of $\mathcal{A}$ whose union is norm-dense in $\mathcal{A}$, then $H_n = [\mathcal{A}_n \xi]$ defines a filtration for which every element of the union $\cup_n \mathcal{A}_n$ has finite degree.

Example 2. Suppose on the other hand that we have an action of $\mathbb{Z}$ on a compact Hausdorff space X for which there is a point $x_0 \in X$ whose orbit under $\mathbb{Z}$ is dense. Then one can write down a representation π of the C^*-algebraic crossed product

$$\mathcal{C} = \mathbb{Z} \times C(X)$$

and a natural filtration for the C^*-algebra $\mathcal{A} = \pi(\mathcal{C})$. To see that, let $\{e_n : n \in \mathbb{Z}\}$ be an orthonormal basis for a Hilbert space H. The representation $\pi_0 : C(X) \to \mathcal{B}(H)$ and the unitary operator $U \in \mathcal{B}(H)$ defined by

$$\pi_0(f)e_n = f(n \cdot x_0)e_n$$
$$Ue_n = e_{n+1}$$

define a covariant pair for the induced action of $\mathbb{Z}$ on $C(X)$, and hence the pair (π_0, U) defines a representation π of the crossed product. Let

$$H_n = [e_{-n}, \dots, e_n], \quad n \geq 1$$

and let $\mathcal{D}$ be the image of $C(X)$ under π_0. It is clear that every element of $\mathcal{D}$ has degree zero, and that $\deg(U) = 1$. Thus any operator expressible as a finite sum

$$A = \sum_{k=-n}^{n} D_k U^k$$

where $D_k \in \mathcal{D}$, has finite degree. Since these operators are dense in $\mathcal{A}$ it follows that $\{H_1 \subseteq H_2 \subseteq \dots\}$ is an $\mathcal{A}$-filtration.

Example 3. Let $\mathcal{T}$ be the Toeplitz C^*-algebra. We represent $\mathcal{T}$ as the C^*-algebra generated by a simple unilateral shift S, acting on an orthonormal basis $\{e_1, e_2, \dots\}$ for H via $Se_n = e_{n+1}$. Let $\mathcal{F} = \{H_n : n \geq 1\}$ be the filtration $H_n = [e_1, e_2, \dots, e_n]$. Notice that $\deg(S) = 1$. Indeed, letting P_n be the projection onto H_n, we have

$$SP_n = P_n S P_n + (P_{n+1} - P_n) S P_n,$$

while $P_n S = P_n S P_n$. Hence $SP_n - P_n S = (P_{n+1} - P_n) S P_n$ is a rank-one operator for every n. It follows that the $*$-algebra $\mathcal{T}_0$ generated by S consists of finite degree operators, and $\mathcal{T}_0$ is dense in $\mathcal{T}$. Thus $\mathcal{F}$ is a $\mathcal{T}$-filtration.

We require the following estimate.

Proposition 4.2. *Let $\mathcal{F} = \{H_n\}$ be a filtration of H, let P_n be the projection onto H_n, and let $A_1, A_2, \dots, A_p$ be a finite set of operators in $\mathcal{B}(H)$. Then for every $n = 1, 2, \dots$ we have*

$$\operatorname{trace}|P_n A_1 A_2 \dots A_p P_n - P_n A_1 P_n A_2 P_n \dots P_n A_p P_n| \leq \|A_1\| \dots \|A_p\| \sum_{k=1}^{p} \deg A_k.$$

proof. Without loss of generality, we can assume that each operator A_k is a contraction and has finite degree. Let us fix n, and define

$$\Delta_p = P_n A_1 A_2 \dots A_p P_n - P_n A_1 P_n A_2 P_n \dots P_n A_p P_n.$$

We claim first that there are contractions $B_1, B_2, \dots, B_p, C_1, C_2, \dots, C_p$ such that

$$\Delta_p = \sum_{k=1}^{p} B_k (\mathbf{1} - P_n) A_k P_n C_k.$$

This is easily seen by induction on p. It is trivial for $p = 1$ (take $B = C = 0$). Assuming it valid for p, we have

$$\Delta_{p+1} = P_1 A_1 \dots A_p (\mathbf{1} - P_n) A_{p+1} P_n + \Delta_p A_{p+1} P_n,$$

and the conclusion is evident from the induction hypothesis on Δ_p.

Each operator $(\mathbf{1} - P_n) A_k P_n$ is of finite rank, since

$$\begin{aligned} \operatorname{rank}((\mathbf{1} - P_n) A_p P_n) &= \operatorname{rank}((\mathbf{1} - P_n)(A_p P_n - P_n A_p)) \\ &\leq \operatorname{rank}(A_p P_n - P_n A_p) \leq \deg A_p \end{aligned}$$

Thus we may write

$$\begin{aligned}\operatorname{trace}|\Delta_p| &\leq \sum_{k=1}^{p} \operatorname{trace}|B_k(\mathbf{1}-P_n)A_kP_nC_k| \\ &\leq \sum_{k=1}^{p} \|B_k\|\|C_k\| \operatorname{trace}|(\mathbf{1}-P_n)A_kP_n| \qquad (4.3) \\ &\leq \sum_{k=1}^{p} \operatorname{trace}|(\mathbf{1}-P_n)A_kP_n|,\end{aligned}$$

where we have used the elementary fact that for any finite rank operator F,

$$\operatorname{trace}|BFC| \leq \|B\|\|C\| \operatorname{trace}|F|.$$

Moreover, for such an F we have

$$\operatorname{trace}|F| \leq \|F\| \cdot \operatorname{rank}(F).$$

Hence

$$\begin{aligned}\operatorname{trace}|(\mathbf{1}-P_n)A_kP_n| \leq \operatorname{rank}((\mathbf{1}-P_n)A_kP_n) &= \operatorname{rank}((\mathbf{1}-P_n)(A_kP_n - P_nA_k)) \\ \leq \operatorname{rank}(A_kP_n - P_nA_k) &\leq \operatorname{deg}A_k.\end{aligned}$$

Utilizing the latter inequality in (4.3) we obtain

$$\operatorname{trace}|\Delta_p| \leq \sum_{k=1}^{p} \operatorname{deg}A_k,$$

as required. □

Let $\mathcal{A}$ be a concrete C^*-algebra. A tracial state of $\mathcal{A}$ is a positive linear functional ρ satisfying $\rho(\mathbf{1}) = 1$ and $\rho(AB) = \rho(BA)$ for every $A, B \in \mathcal{A}$. One might try to construct tracial states of $\mathcal{A}$ by using a filtration $\mathcal{F} = \{H_n : n \geq 1\}$ for H in the following way. Letting P_n be the projection on H_n, we can define a state ρ_n of $\mathcal{B}(H)$ by way of

$$\rho_n(T) = \frac{1}{\dim(H_n)} \operatorname{trace}(P_nT).$$

The restriction of ρ_n to $P_n\mathcal{B}(H)P_n$ is a trace. Of course, ρ_n does not restrict to a trace of $\mathcal{A}$, but one might attempt to obtain a trace by taking weak*-limits of subsequences of $\{\rho_n \restriction_{\mathcal{A}} : n \geq 1\}$, or their averages. In general, this program will fail. It will certainly fail if $\mathcal{A}$ is isomorphic to a Cuntz algebra $\mathcal{O}_n, n = 2, 3, \ldots, \infty$, since $\mathcal{O}_n$ has no tracial states whatsoever. On the other hand, the following result shows that this procedure will succeed when $\mathcal{F}$ is an $\mathcal{A}$-filtration.

Proposition 4.4. *Suppose that $\{H_1 \subseteq H_2 \subseteq \ldots\}$ is an $\mathcal{A}$-filtration. For every $n = 1, 2, \ldots$ put $d_n = \dim H_n$, and let ρ_n be the state of $\mathcal{A}$ defined by*

$$\rho_n(A) = \frac{1}{d_n} \operatorname{trace}(P_nA).$$

Let R_n be the weak-closed convex hull of the set $\{\rho_n, \rho_{n+1}, \rho_{n+2}, \dots\}$. Then $\cap_n R_n$ is a nonempty set of tracial states.*

proof. $R_1, R_2, \dots$ is a decreasing sequence of nonvoid compact convex subsets of the state space of $\mathcal{A}$, and hence the intersection R_∞ is a nonvoid compact convex set of states. We have to show that every element $\sigma \in R_\infty$ is a trace. Since the finite degree elements are dense in $\mathcal{A}$ and σ is bounded, it suffices to show that

$$\sigma(AB) = \sigma(BA)$$

for operators $A, B \in \mathcal{A}$ having finite degree. Because of the inequality

$$|\sigma(AB) - \sigma(BA)| \le \limsup_{n\to\infty} |\rho_n(AB) - \rho_n(BA)|,$$

it suffices to show that $|\rho_n(AB) - \rho_n(BA)| \to 0$ as $n \to \infty$. But since

$$\operatorname{trace}(P_nAP_nBP_n) = \operatorname{trace}(P_nBP_nAP_n)$$

for every n, we may use the case $p = 2$ of Proposition 4.2 as follows

$$\begin{aligned}|\rho_n(AB) - \rho_n(BA)| &= \frac{1}{d_n}|(\operatorname{trace}(P_nABP_n) - \operatorname{trace}(P_nBAP_n)| \\ &\le \frac{1}{d_n}(|\operatorname{trace}(P_nABP_n - P_nAP_nBP_n)| + |\operatorname{trace}(P_nBAP_n - P_nBP_nAP_n)|) \\ &\le \frac{2}{d_n}\|A\|\|B\|(\operatorname{deg}A + \operatorname{deg}B).\end{aligned}$$

The right side obviously tends to 0 as $n \to \infty$ □

Remarks. Given a C^*-algebra $\mathcal{A} \subseteq \mathcal{B}(H)$, it is reasonable to ask if it is always possible to find an $\mathcal{A}$-filtration. Proposition 4.4 implies that *if* an $\mathcal{A}$-filtration exists then $\mathcal{A}$ must have at least one tracial state. Thus, many concrete C^*-algebras cannot be associated with a filtration. For example, if $\mathcal{A}$ is isomorphic to one of the Cuntz algebras $\mathcal{O}_n$, $n = 2, 3, \dots, \infty$, then $\mathcal{A}$ has no tracial states whatsoever, and hence $\mathcal{A}$-filtrations do not exist.

We assume throughout the remainder of this section that $\mathcal{A}$ has a *unique* tracial state τ. Then every self-adjoint operator $A \in \mathcal{A}$ determines a natural probability measure μ_A on $\mathbb{R}$ by way of

$$\int_{-\infty}^{+\infty} f(x)\, d\mu_A(x) = \tau(f(A))$$

for every $f \in C_0(\mathbb{R})$. Clearly the closed support of μ_A is contained in the spectrum of A, and if τ is a faithful trace then we have

$$\operatorname{support}(\mu_A) = \sigma(A).$$

Here is a more explicit description of μ_A. The GNS construction applied to τ gives rise to a representation of $\mathcal{A}$ on another Hilbert space in which the image of $\mathcal{A}$ generates a finite factor M. The spectral measure E_A of A takes values in the projections of M. Letting tr denote the natural normalized trace on M we have

$$\mu_A(S) = \operatorname{tr}(E_A(S))$$

for every Borel set $S \subseteq \mathbb{R}$. The measure μ_A will be called the *spectral distribution* of A.

Assuming now that $\mathcal{F} = \{H_n\}$ is an $\mathcal{A}$-filtration, we have

Theorem 4.5. *Let μ_A be the spectral distribution of a self-adjoint operator $A \in \mathcal{A}$, and let $[a,b]$ be the smallest closed interval containing $\sigma(A)$. For each n, let $d_n = \dim H_n$ and let $\lambda_1, \lambda_2, \dots, \lambda_{d_n}$ be the eigenvalues of $A_n = P_n A \restriction H_n$, repeated according to multiplicity. Then for every $f \in C[a,b]$,*

$$\lim_{n\to\infty} \frac{1}{d_n}(f(\lambda_1) + f(\lambda_2) + \cdots + f(\lambda_{d_n})) = \int_a^b f(x)\, d\mu_A(x).$$

proof. Let τ_n be the state of $\mathcal{B}(H)$ defined by

$$\tau_n(T) = \frac{1}{d_n}\mathrm{trace}(P_n T).$$

Noting that τ_n restricts to the normalized trace on $P_n\mathcal{B}(H)P_n$, Theorem 4.5 will become evident once we have established the following two assertions.

(i) For every $f \in C[a,b]$, we have

$$\lim_{n\to\infty} |\tau_n(f(A)) - \tau_n(f(P_nAP_n))| = 0.$$

(ii) For every $B \in \mathcal{A}$,

$$\lim_{n\to\infty} \tau_n(B) = \tau(B),$$

where τ is the tracial state of $\mathcal{A}$.

To prove (i), notice that since the sequence of linear functionals

$$f \in C[a,b] \mapsto \tau_n(f(A)) - \tau_n(f(P_nAP_n))$$

is uniformly bounded (an upper bound for their norms is 2), it is enough to prove (i) for polynomials f; and by linearity, we may further reduce to the case where f is a monomial, $f(x) = x^p$ for some $p = 1, 2, \dots$. Finally, since the sequence of p-linear forms

$$B_n(T_1, T_2, \dots, T_p) = \tau_n(T_1T_2 \dots T_p) - \tau_n(P_nT_1P_nT_2P_n \dots P_nT_pP_n)$$

is uniformly bounded (again, $\|B_n\| \le 2$), it is enough to prove that

$$\lim_{n\to\infty} |\tau_n(A^p) - \tau_n((P_nAP_n)^p)| = 0$$

for operators A having finite degree. But in this case, Proposition 4.2 implies that

$$|\tau_n(A^p) - \tau_n((P_nAP_n)^p)| \le \frac{p}{d_n}\|A\|^p \deg(A),$$

and the right side obviously tends to 0 as $n \to \infty$.

Assertion (ii) follows immediately from Proposition 4.4. For if R_n denotes the sequence of convex sets of 4.5, then their intersection must consist of the singleton $\{\tau\}$; hence the sequence of states

$$B \in \mathcal{A} \mapsto \tau_n(B) = \frac{1}{d_n}\mathrm{trace}(P_nB)$$

has a unique weak* cluster point τ, hence it must actually converge to τ in the weak* topology □

Remark 4.6. Let $A = A^* \in \mathcal{A}$. If one drops the hypothesis that $\mathcal{A}$ has a unique trace, then the averages of the eigenvalues of $P_nA \restriction H_n$ may fail to converge. However, one can push the method of proof to obtain other useful conclusions in certain cases. For example, if we assume that there are *sufficiently many* traces in the sense that for every nonzero $B \in \mathcal{A}$ there is a tracial state τ such that $\tau(B^*B) > 0$, then one can obtain the following information about the density of eigenvalues in the vicinity of a point of the spectrum of A. Let $N_n(U)$ denote the number of eigenvalues of $P_nA \restriction H_n$ which belong to the open set U, and let λ be a point in the spectrum of A. Then for every neighborhood U of λ there is a positive number ϵ such that

$$\frac{N_n(U)}{\dim(H_n)} \geq \epsilon,$$

for all sufficiently large n. We omit the details since this result is not relevant to our needs below.

5. Applications.

Most one-dimensional quantum mechanical systems are described by a Hamiltonian which is a densely defined unbounded self-adjoint operator on $L^2(\mathbb{R})$, having the form

$$Hf(x) = -\frac{1}{2}f''(x) + V(x)f(x)$$

$V : \mathbb{R} \to \mathbb{R}$ being a continuous function representing the potential. If one wishes to simulate the behavior of such a quantum system on a computer, one first has to discretize this differential operator in an appropriate way. Secondly, one has to develop effective methods for computing with the discretized Hamiltonian. For our purposes, we interpret the second goal to be that of computing the spectrum.

In [1], [2], we discussed the problem of discretizing the above Hamiltonians in such a way as to preserve the uncertainty principle. We argued that the appropriate discretization is a bounded self-adjoint operator of the form

$$H_\sigma = -\frac{1}{2}P_\sigma^2 + V(Q_\sigma) \tag{5.1}$$

where P_σ and Q_σ are the bounded self-adjoint operators given by

$$P_\sigma f(x) = \frac{1}{2i\sigma}(f(x+\sigma) - f(x-\sigma)),$$
$$Q_\sigma f(x) = \frac{1}{\sigma}\sin(\sigma x)f(x).$$

Here, σ is a small (positive rational) number representing the numerical step size.

In even the simplest cases, one cannot carry out explicit calculations of the spectrum of the discretized Hamiltonians 5.1 (see [3],[4],[5],[7],[9]). On the other hand, one can apply the methods of the prceding sections in a straightforward manner to obtain the spectrum of H_σ as the limiting case of finite dimensional eigenvalue distributions.

To see this, let U and V be the unitary operators

$$\begin{aligned} Uf(x) &= e^{i\sigma x} f(x), \\ Vf(x) &= f(x + 2\sigma). \end{aligned}$$

Then 5.1 can be written in the form $H_\sigma = \alpha A + \beta \mathbf{1}$, where α and β are real numbers and A is a bounded self-adjoint operator of the form

$$A = V + V^* + v\left(\frac{1}{2i}(U - U^*)\right). \tag{5.2}$$

Here, $v : \mathbb{R} \to \mathbb{R}$ is an appropriately rescaled version of V. Thus, we are interested in the spectrum of A. Of course, A belongs to the C^*-algebra $C^*(U, V)$ generated by U and V. Following the program outlined in section 4, we will first find a faithful representation of $C^*(U, V)$ in which there is a compatible filtration, and then we will look at the eigenvalues fo the approximating sequence of finite matrices. Since U and V obey the commutation relation

$$VU = e^{2i\sigma^2} UV \tag{5.3}$$

and since σ is a rational number, it follows that $C^*(U, V)$ is an irrational rotation C^*-algebra. Thus in order to define a faithful representation, it is enough to specify a pair of unitary operators U_1 and V_1 which satisfy the same commutation relation 5.3. For that, consider a Hilbert space spanned by an orthonormal basis $\{e_n : n \in \mathbb{Z}\}$ and define U_1 and V_1 by

$$\begin{aligned} U_1 e_n &= e^{-2in\sigma^2} e_n, \\ V_1 e_n &= e_{n+1}. \end{aligned}$$

The pair $\{U_1, V_1\}$ is irreducible, it obeys the required commutation relations, and A becomes the tridiagonal operator $V_1 + V_1^* + D$, where D is the diagonal operator

$$De_n = v(-\sin(2\sigma^2 n))e_n, \qquad n \in \mathbb{Z}.$$

Let $\mathcal{A} = C^*(U_1, V_1)$. Then the sequence of subspaces $H_1, H_2, \dots$ defined by $H_n = [e_{-n}, e_{-n+1}, \dots, e_n]$ is an $\mathcal{A}$-filtration (see example 2 of section 4). Since concretely represented irrational rotation C^*-algebras never contain nonzero compact operators, the spectrum of A coincides with the essential spectrum of A. Moreover, by Theorem 3.8, the spectrum of A is the set of essential points associated with the sequence of matrices $\{A_n : n \geq 1\}$, A_n being the compression of A to H_n. The remaining points of Λ are all transient points. Finally, since irrational rotation C^*-algebras are simple and have a unique trace, we may conclude from Theorem 4.5 that for every $f \in C_0(\mathbb{R})$ one has the following convergence of the densities of eigenvalues,

$$\lim_{n\to\infty} \frac{1}{2n+1}(f(\lambda_1) + \cdots + f(\lambda_{2n+1})) = \int_{-\infty}^{+\infty} f(x)\, d\mu_A(x), \tag{5.1}$$

wehre μ_A is the spectral distribution of A and $\{\lambda_1, \dots, \lambda_{2n+1}\}$ is the eigenvalue list of A_n.

We remark that this representation is particularly convenient for numerical eigenvalue computations using the QL or QR algorithms, because the matrices $A_1, A_2, \dots$ are already in tridiagonal form relative to the obvious basis.

6. Appendix. Failure of $\sigma_e(A) = \Lambda_e$. In this section we give an example of a self-adjoint operator A on a Hilbert space spanned by an orthonormal basis $\{e_1, e_2, \dots\}$, such that the relation of A to the filtration $H_n = [e_1, e_2, \dots, e_m]$, $n = 1, 2, \dots$ is pathological. We show that if A_n is the compression of A to H_n, then Λ_e contains points not in the spectrum of A, and in particular $\Lambda_e \neq \sigma_e(A)$.

Specifically, A is a reflection (i.e., a self-adjoint unitary operator) whose essential spectrum is $\{-1, +1\}$, whereas $0 \in \Lambda_e$. In the example $H = l^2(\mathbb{N})$, e_n is the unit coordinate funtion at n, and A will be the operator in $l^2(\mathbb{N})$ induced by a permutation π of $\mathbb{N}$ satisfying $\pi^2 = \mathrm{id}$. Let I_n denote the interval $\{1, 2, \dots, n\}$, and let $\#S$ denote the number of elements of a set S. Suppose further that the permutation π has the following property

$$\lim_{n\to\infty} \#(\pi(I_n) \setminus I_n) = +\infty. \tag{A.1}$$

For each $n \geq 1$, let A_n be the compression of the operator $A\xi(k) = \xi(\pi(k))$ to $H_n = l^2(I_n)$. Since A maps e_k to $e_{\pi(k)}$, it follows that for every k in the set $S_n = \{k \in I_n : \pi(k) \notin I_n\}$, we have $A_n e_k = 0$. Since the cardinality of S_n tends to infinity, it follows that 0 is an eigenvalue of every A_n and that the multiplicity of this zero eigenvalue tends to infinity. Hence, 0 must belong to Λ_e.

Thus it suffices to exhibit an order two permutation having the property A.1. Let E and O denote respectively the set of even and odd integers in $\mathbb{N}$. In order to define a permutation π with $\pi^2 = \mathrm{id}$, it is enough to specify a bijection $f : E \to O$; once we have f then we can define π by

$$\pi(k) = \begin{cases} f(k), k \in E \\ f^{-1}(k), k \in O. \end{cases}$$

We will define a bijection $f : E \to O$ having the following property with respect to the initial intervals I_n:

$$\lim_{n\to\infty} \#(f(E \cap I_n) \setminus I_n) = +\infty. \tag{A.2}$$

The resulting permutation will have the desired property A.1.

To construct f, split E into two disjoint subsets $E_1 \cup E_2$, where $E_1 = 4\mathbb{N}$ is the set of multiples of 4 and E_2 is the rest. Both E_1 and E_2 are infinite of course. First define f on E_1 by

$$f(k) = k^2 + 1. \tag{A.3}$$

Let $O_1 = f(E_1)$, and put $O_2 = O \setminus O_1$. Noting that O_2 is infinite (everything in O_1 is congruent to 1 mod 16, hence O_2 contains all the other odd numbers), we can complete the definition of f by choosing it to be any bijection of E_2 onto O_2.

To prove A.2, it suffices to show that $\#(f(E_1 \cap I_n) \setminus I_n)$ tends to infinity with n. Noting that

$$E_1 \cap I_n = \{4k : 1 \leq k \leq [n/4]\},$$

we see that

$$f(E_1 \cap I_n) = \{16k^2 + 1 : 1 \leq k \leq [n/4]\}$$

Thus every element in the subset P_n of $E_1 \cap I_n$ defined by

$$P_n = \{4k : \frac{\sqrt{n}}{4} < k \le \frac{n}{4}\}$$

gets mapped by f into the complement of I_n. Hence

$$\#(f(E_1 \cap I_n) \setminus I_n) \ge \# P_n \ge \frac{n}{4}(1 - n^{-1/2}).$$

This estimate implies that $\#(f(E \cap I_n) \setminus I_n) \to \infty$, and A.2 follows.

Remark. Notice that this misbehavior cannot be corrected by averaging the eigenvalues of A_n as we did in section 4. Indeed, if $N_n(U)$ denotes the number of eigenvalues of A_n which belong to an open set U, then the above estimate shows that for every neighborhood U of 0 we have

$$\liminf_{n\to\infty} \frac{N_n(U)}{\dim H_n} \ge \frac{1}{4} > 0,$$

in spite of the fact that 0 does not belong to the spectrum of A.

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